

U.S.-JAPAN SEMINAR ON EVALUATION, COMPILATION, AND  
PRESENTATION OF PHYSICAL PROPERTY DATA AND DATA CENTER ACTIVITIES

Tokyo, Japan  
November 15-17, 1971

I. INTRODUCTION

A Seminar on Evaluation, Compilation, and Presentation of Physical Property Data and Data Center Activities was held under the auspices of the Science and Technology Agency of Japan and the National Science Foundation, as an activity of the United States-Japan Scientific Cooperation Program in its Category 3 - Scientific Communication. Its stated purpose was to bring together scientists from the two countries who are concerned with evaluation and dissemination of physical property data, in order that they might exchange information on current activities and explore possibilities for mutually beneficial cooperation. The seminar lasted three days and included 23 formal lectures plus extensive discussion, as well as numerous informal meetings.

The full list of participants is given below. The U.S. Delegation was made up principally of individuals who have been associated in some way with the National Standard Reference Data System. The Japanese Delegation included several who have been involved with data evaluation groups in the U.S. or with international groups such as CODATA. There was a strong representation of chemists among the Japanese, as well as a number of mechanical engineers. Physics, especially the nuclear area, seemed under-represented.

II. LIST OF PARTICIPANTS

U.S. DELEGATION - Dr. Allen V. Astin, Coordinator

1. Dr. Allen V. Astin  
Director Emeritus  
National Bureau of Standards
2. Dr. Edward L. Brady  
Associate Director for Information Programs  
National Bureau of Standards
3. Dr. D. Garvin  
Coordinator for Data Evaluation Programs  
Physical Chemistry Division  
Institute for Materials Research  
National Bureau of Standards
4. Dr. L. J. Kieffer  
Astrophysics Division  
Boulder Laboratories  
National Bureau of Standards
5. Dr. H. William Koch  
Director  
American Institute of Physics
6. Dr. D. R. Lide, Jr.  
Chief, Office of Standard Reference Data  
National Bureau of Standards
7. Dr. Y. S. Touloukian  
Director  
Thermophysical Properties Research Center  
Distinguished Atkins Professor of Engineering  
School of Mechanical Engineering
8. Dr. D. D. Wagman  
Physical Chemistry Division  
Institute for Materials Research  
National Bureau of Standards
9. Prof. E. F. Westrum, Jr.  
Department of Chemistry  
University of Michigan

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PARTICIPANTS FROM OTHER COUNTRIES

1. Dr. R. N. Jones  
National Research Council  
CANADA

JAPANESE DELEGATION - Dr. Masao Kotani, Coordinator

1. Prof. Hideaki Chihara  
Department of Chemistry  
Osaka University
2. Prof. Soshin Chikazumi  
Institute for Solid State Physics  
University of Tokyo
3. Prof. Shizuo Fujiwara  
Department of Chemistry  
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4. Prof. Mitsuho Hirata  
Department of Chemical Engineering  
Tokyo Metropolitan University
5. Dr. Kenzo Hirayama  
Director  
Technical Information Service  
Fuji Photo Film Co., Research Laboratory
6. Prof. Sukeaki Hosoya  
Institute for Solid State Physics  
University of Tokyo
7. Dr. Tomoyoshi Kawada  
Director  
National Research Institute for Metals
8. Prof. Yuichi Kawada  
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9. Prof. Koreo Kinoshita  
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10. Prof. Shotaro Kodama  
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11. Dr. Masao Kotani  
President  
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12. Prof. Kozo Kuchitsu  
Department of Chemistry  
University of Tokyo
13. Prof. Tadashi Makita  
Department of Chemical Engineering  
Kobe University
14. Dr. Yo-ichiro Mashiko  
Director  
National Chemical Research Institute for Industry
15. Prof. Akira Nagashima  
Department of Mechanical Engineering  
Keio University
16. Prof. Jiro Osugi  
Department of Chemistry  
Kyoto University
17. Prof. Takehiko Shimanouchi  
Department of Chemistry  
University of Tokyo
18. Prof. Yoshio Takeuchi  
Mineralogical Institute  
University of Tokyo
19. Prof. Ichimatsu Tanishita  
Department of Mechanical Engineering  
Keio University
20. Prof. Mitsuo Tasumi  
Department of Biophysics and Biochemistry  
University of Tokyo
21. Dr. Toshikazu Tsuchiya  
Head, Second Division  
National Chemical Research Institute for Industry
22. Prof. Koichi Watanabe  
Department of Mechanical Engineering  
Keio University
23. Dr. Susumu Yoshida  
Head, Materials Testing Division  
National Research Institute for Metals

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24. Prof. Yasuhide Yukawa  
Institute of Scientific and Industrial Research  
Osaka University

OBSERVERS AND STAFF

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American Embassy, Tokyo
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6. Dr. Michio Kawata  
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Research Planning Director  
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8. Mr. Masaji Sawabe  
Principal Research Officer Laboratory of Metrology
9. Miss Teruko Inamatsu  
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National Research Laboratory of Metrology
10. Prof. Tatsuo Miyazawa  
Institute for Protein Research  
Osaka University

11. Prof. Takashi Shimozawa  
Department of Chemistry  
Saitama University

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1. Prof. Masamichi Tsuboi  
Faculty of Pharmaceutical Sciences  
University of Tokyo
2. Prof. Ichiro Nakagawa  
Department of Chemistry  
University of Tokyo

MEMBER OF EXECUTIVE COMMITTEE OF IRDC

1. Dr. Shigeru Yamauchi  
Department of Industrial Chemistry  
University of Tokyo
2. Dr. Tomoko Nakahara  
Department of Chemical Engineering  
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3. Miss Derothy U. Mizoguchi  
Chief  
Cancer Chemotherapy Information Center

SCIENCE AND TECHNOLOGY AGENCY

1. Mr. Yoshiro Narabayashi  
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Head of Administration Division  
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9. Mr. Takashi Hironaka  
Chief of Information Section  
Promotion Bureau

### III. PROGRAM

MONDAY - November 15, 1971

Morning: Session 1 (10:00 a.m. - 12:00 noon)

1. Welcome Address by Representative of Japanese  
Implementing Agency

Mr. Yoshiro Narabayashi  
Director General  
Planning Bureau  
Science and Technology Agency

2. Addresses by Representative of Participants  
from Japan and U.S.

Dr. M. Kotani  
President  
Science University of Tokyo

Dr. A. V. Astin  
Director Emeritus  
National Bureau of Standards

3. Adoption of Agenda
4. Presentation and Discussion of Papers  
(1) Data Handling in Primary Publications in Japan

Prof. H. Chihara  
Department of Chemistry  
Osaka University

Executive Secretary  
Japanese CA Abstractors Association

- (2) Presentation of Concepts and Numerical Data  
in Physics

Dr. H. William Koch  
Director  
American Institute of Physics

Afternoon: Session 2 (2:00 - 5:00 p.m.)

- (3) Rationale and Development of the U.S. National  
Standard Reference Data System

Dr. Edward L. Brady  
Associate Director for Information Programs  
National Bureau of Standards

- (4) Present Status of the U.S. Standard Reference  
Data Program

Dr. D. R. Lide, Jr.  
Chief, Office of Standard Reference Data  
National Bureau of Standards

- (5) Data Center Activity on Molecular Vibrations

Prof. T. Shimanouchi  
Department of Chemistry  
University of Tokyo

- (6) Collection and Evaluation of Molecular Vibrational Frequencies

Prof. M. Tasumi  
Department of Biophysics and Biochemistry  
University of Tokyo

- (7) Functions of High Pressure Data Center

Prof. J. Osugi  
Department of Chemistry  
Kyoto University



TUESDAY - November 16, 1971

Morning: Session 3 (9:30 a.m. - 12:00 noon)

- (8) The Thermophysical Properties Research Center  
Its Aims and Activities

Dr. Y. S. Touloukian  
Director  
Thermophysical Properties Research Center  
Distinguished Atkins Professor of Engineering  
School of Mechanical Engineering

- (9) Evaluation of Experimental Data for Thermodynamic  
Properties of Fluorocarbon Refrigerants

Prof. I. Tanishita  
Prof. K. Watanabe  
Division of Mechanical Engineering  
Keio University

- (10) Critical Evaluation of Data in Chemical Thermodynamics

Dr. D. D. Wagman  
Physical Chemistry Division  
Institute for Material Research  
National Bureau of Standards

- (11) Collection of Data on Fatigue Strength of Metals  
and the Need of Their Statistical Treatment

Prof. Y. Kawada  
Department of Mechanical Engineering  
Tokyo Metropolitan University

Afternoon: Session 4 (2:00 - 5:00 p.m.)

- (12) Collection and Evaluation of Electron Diffraction Data

Prof. K. Kuchitsu  
Department of Chemistry  
University of Tokyo

- (13) Measurement Techniques and the Evaluation of Property Data

Dr. L. J. Kieffer  
Astrophysics Division  
Boulder Laboratories  
National Bureau of Standards

(14) Evaluation of X-ray Diffraction Data

Prof. S. Hosoya  
Institute for Solid State Physics  
University of Tokyo

(15) Criteria for Reporting Property Measurements in  
the Literature

Prof. E. F. Westrum, Jr.  
Department of Chemistry  
University of Michigan

(16) Present Status of Activities for Collection and  
Distribution of Mass Spectral Data in Japan

Dr. T. Tsuchiya  
Head  
Second Division  
National Chemical Research Institute for Industry

WEDNESDAY - November 17, 1971

Morning: Session 5 (9:30 a.m. - 12:00 noon)

(17) Computer Storage and Search of Spectral Data

Dr. R. N. Jones  
National Research Council  
Canada

(18) Long-Term Creep Data on Domestic Materials Obtained at  
National Research Institute for Metals

Dr. T. Kawada  
Director  
National Research Institute for Metals

Dr. S. Yoshida  
Head  
Materials Testing Division  
National Research Institute for Metals

(19) Complete Clear Text Representation of Scientific Documents  
in Machine-Readable Form

Dr. D. Garvin  
Coordinator for Data Evaluation Programs  
Physical Chemistry Division  
Institute for Materials Research  
National Bureau of Standards

- (20) Compilation and Computer Estimation of Physical Property Values for Chemical Engineers

Prof. M. Hirata  
Department of Chemical Engineering  
Tokyo Metropolitan University

Afternoon: Session 6 (2:00 - 5:00 p.m.)

- (21) A Plan of Data Depository Center for Organic Chemistry

Prof. Y. Yukawa  
Institute of Scientific and Industrial Research  
Osaka University

- (22) Necessity of Establishing Data (Service) Center in Japan

Dr. Y. Mashiko  
Director  
National Chemical Research Institute for Industry

- (23) Opportunities for U.S. - Japan Cooperative Projects

Dr. D. R. Lide, Jr.  
Chief, Office of Standard Reference Data  
National Bureau of Standards

#### IV. SUMMARY OF U.S. PAPERS

The papers presented by the U.S. Delegation fell into three categories: data evaluation under the NSRDS program, reporting of data in the primary literature, and the use of computers in data processing. The background of the National Standard Reference Data System and the philosophy of its operation were described by E. L. Brady, and current activity under the program was summarized by D. R. Lide. Particular emphasis was given to problems of dissemination of reference data. D. D. Wagman discussed the procedures followed by the Chemical Thermodynamics Data Center in evaluating

a large ensemble of highly interrelated data. There was also a discussion of the activity of CODATA in establishing standard values of thermodynamic properties of key substances. A different aspect of the evaluation problem was described by L. J. Kieffer, who stressed the difficulty in assessing the contribution of various sources of systematic error. The importance of having a thoroughly understood and completely documented theory of the experiment was brought out in this talk. Y. S. Touloukian discussed the problems of operating a large information analysis center in which information retrieval, data evaluation, and experimental and theoretical research are highly integrated.

Some aspects of the presentation of results of experimental measurements were discussed by two speakers. H. W. Koch described plans of the American Institute of Physics to develop more effective means of distributing primary and secondary information to the physics community. E. F. Westrum stressed the need for more complete reporting of the results of experimental measurements in the primary literature. He described the work of thermodynamicists in drawing up a "Guide to the Publication of Thermodynamic Data" which gives detailed instructions on the way in which data should be reported and the auxiliary information which should be supplied.

The role of modern computers in data handling was discussed by two speakers. R. N. Jones (who was present as a third-country representative from Canada) discussed the computer storage and retrieval of spectral data. He stressed the importance of setting uniform formats for reporting spectral data of all types and for insuring the technical quality of the data before

it went into a computer storage bank. D. Garvin described the General Purpose Scientific Document Image Code, a system for storing scientific data and text in a manner which permits great flexibility of output.

#### V. SUMMARY OF JAPANESE PAPERS

Although most of the Japanese papers dealt with specific technical areas, three speakers covered more general problems. H. Chihara discussed the presentation of data in the primary literature, stressing the need for journal editors to exert better quality control over the papers which they publish. He also described efforts in Japan to make original experimental data available to evaluators when it is too bulky to publish in regular journals. There was also a discussion of Japanese contributions to the preparation of abstracts for Chemical Abstracts.

A proposal for establishing a large data distribution center in Japan was presented by Y. Mashiko. The center would collect and index data compilations from all parts of the world and maintain contact with data evaluation centers. Inquiries for data and other information would be answered from the resources of the center. Y. Yukawa described plans for an organic chemistry data depository center. This center would collect data of various types -- spectral, thermodynamic, physical properties, etc. -- classified by compound and make it available to inquirers. The aim appeared to be to establish a comprehensive, but not necessarily critical depository, although cooperation with data evaluation centers was mentioned. Neither of these proposals seemed to have reached the stage of concrete planning,

especially as regards financial considerations.

Data evaluation activities in several specific technical areas were described by the other Japanese participants. Vibrational spectroscopy was covered by T. Shimanouchi and M. Tasumi. They discussed the Japanese collection of infrared spectral data (IRDC), bibliographic activities on infrared and Raman spectroscopy, collections of force constants, and the preparation of tables of molecular vibrational frequencies. The latter project is carried out as part of the NSRDS program. T. Tsuchiya discussed mass spectral data and outlined the way in which Japanese activities fitted into the international program on mass spectral data collection. A Japanese group has published three annual indices to the literature of organic mass-spectra, but the project has encountered financial difficulties. There were two talks in the area of molecular structure. K. Kuchitsu discussed structural data obtained by gas-phase electron diffraction; he described existing bibliographic activities and pending evaluation projects of an international nature. In view of the great research activity in this field in Japan, a strong input to compilation and evaluation is hoped for. Evaluation of X-ray diffraction data on solids was discussed by S. Hosoya. Here Japanese groups have been cooperating with other national and international groups in standardizing measurements and developing data files.

J. Osugi described the High Pressure Data Center of Japan, which works closely with its U.S. equivalent at Brigham Young University. These two groups exchange information on high pressure phenomena on a regular basis.

Evaluation of equation of state data on fluorocarbon refrigerants was described in some detail by I. Tanishita, K. Watanabe, H. Kondo, and K. Oguchi. Japanese efforts on properties of fluids of interest to chemical engineers were outlined by M. Hirata. These include publication of an annual summary of physical properties retrieved from the primary literature and development of a computer program for estimation and retrieval of property data.

Finally, two papers were devoted to mechanical property data. Y. Kawada discussed the collection of data on the fatigue strength of metals, stressing particularly the need for a statistical approach because of the variability found over a range of samples. A program for collecting long-term creep data on structural materials was described by T. Kawada and S. Yoshida. In its present form, this involves testing of samples in a central laboratory under standardized procedures. Data sheets will be published annually beginning in 1972.

#### VI. SUMMARY AND PROGNOSIS FOR FUTURE COOPERATION

It is evident from the above outline of the symposium that there is considerable data compilation activity in Japan, but that the coverage of technical areas is rather spotty. In the absence of any central coordinating body, data centers and other evaluation activities have grown up on the initiative of individual Japanese scientists, often with influence from foreign groups. The difficulty in obtaining stable funding, or even clear directives, from government or industry is apparent. Several

projects appeared to suffer from inadequate funding, and some publication series had ceased after the first two or three years. On the other hand, there seemed to be a strong market for data and other technical information in Japan; the circulation figures for some of the publications mentioned at the symposium were quite impressive.

All of the Japanese participants seemed to feel, not surprisingly, that the Japanese Government should provide more funds for data compilation and evaluation. However, there were a variety of views on the way these funds should be spent. Some participants hoped for more support for individual data evaluation projects, particularly in the universities. Interest was expressed in setting up data centers, on the NSRDS model, in a number of technical areas. Other speakers emphasized the need for funds for a central service organization, covering a broad scope, which would respond to requests for data.

One point which emerged from the symposium was that a significant amount of U.S.-Japanese cooperation already exists in the data field. Examples of activities in which Japanese and U.S. groups cooperate on a regular basis include:

1. Molecular vibrational frequencies - T. Shimanouchi, University of Tokyo compiles data for publication in the NSRDS series.
2. Thermochemistry - Y. Takahashi, University of Tokyo, contributes to the Annual Bulletin of Thermodynamics and Thermochemistry, edited by E. F. Westrum, University of Michigan.
3. Viscosity and specific heat - T. Makita, Kobe University, evaluates data for Thermophysical Properties Research Center, Purdue University.



4. High pressure data - J. Osugi, Kyoto University, exchanges information with High Pressure Data Center, Brigham Young University.
5. Molecular structure - bibliography on gas phase molecular structure is being prepared as multi-national effort to which K. Kuchitsu, University of Tokyo, and W. H. Kirchhoff, National Bureau of Standards are making major input.

These and other examples of working cooperation have developed spontaneously as a result of a confluence of interests on the part of individual scientists in the two countries. Some of the arrangements have been operating very effectively for a number of years.

If a formal data program is established by the Japanese Government in the future, there will undoubtedly be increased opportunities for collaboration. From the viewpoint of cooperation at the planning level, it would be desirable to have a central focal point in Japan similar to the NBS Office of Standard Reference Data in the U.S. We could establish procedures for routine exchange of information, exchange of proposals for review, and take other steps to insure against unnecessary duplication of effort. An interaction of this type between the Office of Standard Reference Data and the Office of Scientific and Technical Information (OSTI) in the United Kingdom has proved very effective. A similar arrangement between the U.S. and Japan should be helpful to both sides.

In addition to the areas listed above where substantive collaboration between U.S. and Japanese groups already exists, several other possibilities for joint projects presented themselves during the symposium. Among the more promising areas are:

1. Interatomic distances - There is strong interest and considerable competence in Japan in the determination of interatomic distances by diffraction and spectroscopic methods. An international effort to prepare tables of evaluated structural data has been proposed. It is reasonable to expect the U.S. and Japan to play a major part.
2. Thermodynamic properties of fluids - Possibilities for collaboration under various international programs.
3. Mechanical properties - Activities planned in U.S. might be coordinated with existing Japanese program.
4. Magnetic properties of solids - There is interest in Japan in starting compilation in this area, where there is now little activity in the U.S.
5. Nuclear magnetic resonance - Interest in compilation projects exists in both countries. This is a very large area, which could usefully be partitioned.
6. Photochemistry - This is an active research field in Japan, and data program might be developed which would mesh with chemical kinetics program in the U.S.

Other areas such as mass spectroscopy, gas chromatography, and infrared spectroscopy also offer possibilities for joint projects. On a different level, the present arrangement for providing abstracts from the Japanese literature to Chemical Abstracts might be extended to other disciplines. Finally, it seems desirable to consult on computer formats for handling

data. Adoption of common formats at an early stage will simplify data exchange between centers in the two countries.

Extended abstracts of the papers presented at the Symposium are attached.



REPORT SUBMITTED BY: Dr. David R. Lide, Jr., Chief  
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March 27, 1972